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14. ABSTRACT

We present a new algorithm for the retrieval of kinetic temperature in the terrestrial mesosphere and lower thermosphere from measurements of CO_2 15 μm earth limb emission. Non-local-thermodynamic-equilibrium (non-LTE) processes are rigorously included in the new algorithm, necessitated by the prospect of satellite-based limb radiance measurements to be made from the TIMED/SABER platform in the near future between 15 km and 120 km tangent altitude. The algorithm requires 20 seconds to retrieve temperature to better than 3 K accuracy on a desktop computer, easily enabling its use in operational processing of satellite data. We conclude this letter with a study of the sensitivity of the retrieved temperatures to parameters used in the non-LTE models, including sensitivity to the rate constant for physical quenching of CO_2 bending mode vibrations by atomic oxygen.

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Retrieval of mesospheric and lower thermospheric kinetic temperature from measurements of CO_2 15 μm Earth limb emission under non-LTE conditions

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Abstract. We present a new algorithm for the retrieval of kinetic temperature in the terrestrial mesosphere and lower thermosphere from measurements of CO_2 15 μm earth limb emission. Non-local-thermodynamic-equilibrium (non-LTE) processes are rigorously included in the new algorithm, necessitated by the prospect of satellite-based limb radiance measurements to be made from the TIMED/SABER platform in the near future between 15 km and 120 km tangent altitude. The algorithm requires 20 seconds to retrieve temperature to better than 3 K accuracy on a desktop computer, easily enabling its use in operational processing of satellite data. We conclude this letter with a study of the sensitivity of the retrieved temperatures to parameters used in the non-LTE models, including sensitivity to the rate constant for physical quenching of CO_2 bending mode vibrations by atomic oxygen.

Introduction

Techniques to retrieve temperature profiles from broadband measurements of CO_2 15 μm earth limb emission from the middle atmosphere were developed more than 30 years ago (e.g., [*Gille and House*, 1971]). In these techniques a basic assumption was that carbon dioxide (CO_2) was well mixed and its volume mixing ratio (vmr) was well known. Another key assumption was that the observed CO_2 transitions were in LTE. These assumptions were sufficient for previous sensors whose sensitivity did not permit limb radiance measurements much above 70 km tangent height.

In the very near future, NASA will launch and commence operations of the Thermosphere-Ionosphere-Mesosphere Energetics and Dynamics (TIMED) mission whose primary goals are to measure the thermal structure and to quantify the energy budget of the 60-180 km region. One TIMED instrument, SABER (Sounding of the Atmosphere using Broadband Emission Radiometry), will measure CO_2 limb emission in the 15 μm spectral interval to approximately 120 km in altitude for the purpose of determining kinetic temperature (T_k). SABER is a broadband radiometer with 10 spectral channels ranging from 1.27 μm to 16 μm. To analyze the SABER limb radiance data in terms of T_k, new retrieval approaches must be developed to deal effectively with the occurrence of non-LTE in the observed vibration-rotation bands of CO_2 as well as variability in the CO_2 vmr. The purpose of this letter is to present the algorithm for retrieving T_k from non-LTE emission measurements and to present the sensitivity of the retrievals to parameters in the non-LTE model.

Temperature retrieval approach

Kinetic temperature is retrieved using SABER measured radiance from two CO_2 15 μm channels, a narrow bandpass channel (650-695 cm^{-1}) and a wide bandpass channel (580-760 cm^{-1}). The two CO_2 channels are used to register pressure with altitude in the stratosphere and infer T_k assuming LTE conditions. This approach is similar to the two-color technique of *Gille and House* [1971]. The LTE assumption breaks down in the mesosphere for the CO_2 15 μm bands. The non-LTE retrieval algorithm is then employed to infer T_k in the mesosphere and lower thermosphere (MLT) using measured radiance from the CO_2 narrow channel.

The LTE-retrieved T_k and pressure described in the preceding paragraph provide the lower boundary conditions for the non-LTE T_k retrieval. The lower boundary altitude is nominally taken to be 50 km.

The non-LTE T_k retrieval model is comprised of two main components: (1) the forward radiance model and (2) the inversion model. Moreover, the forward radiance

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model itself is composed of two parts: (1) the vibrational temperature (T_v) model and (2) the limb radiance model. Limb radiance is calculated using BANDPAK [*Marshall et al.*, 1994], now expanded for applications to non-LTE calculations. There are seventeen 15 μm bands that contribute to the limb radiance in the CO_2 narrow channel spectral bandpass. Vibrational temperatures for these seventeen bands are the non-LTE inputs into the limb radiance model. The non-LTE formulation in BANDPAK is a broadband extension of the line-by-line approach described by *Edwards et al.* [1993] and demonstrated by *Mlynczak et al.* [1994]. The vibrational temperatures are calculated from the operational CO_2 T_v model, which is a formulation of the Modified Curtis Matrix approach of *López-Puertas et al.* [1998a] that uses BANDPAK to perform all the radiation transfer calculations.

A number of techniques are used in the inversion model of the retrieval algorithm. There are two primary relaxation loops. In the inner loop a T_k profile is retrieved using the onion-peel approach while pressure and the T_v's are fixed. The onion-peel technique is characterized by first matching the emission of the outer atmospheric layer to the measured radiance, then successively matching the next inward layer. Kinetic temperature is retrieved at each tangent height by adjusting the local T_k until the modeled radiance matches the measured radiance within the convergence criterion. The temperature is adjusted using Newtonian iteration and the optimal estimation algorithm [*Rodgers*, 1976]. The inner loop convergence criterion is a requirement that the modeled radiance match the measured radiance within a user-specified fraction of the solution error (standard deviation).

The onion-peel approach is critical to retrievals in the mesosphere from the CO_2 15 μm bands since the limb radiance for mesospheric tangent heights is dominated by emission from higher altitude layers [*Wintersteiner et al.*, 1992]. The onion-peel technique ensures that the modeled emission matches the measured radiance from the upper altitude layers, even though the retrieved temperature-pressure combination may be incorrect at intermediate steps in the relaxation process. For a particular limb path, the effect is greater sensitivity to the local T_k at the sought-after tangent altitude.

Operationally, the *a priori* temperature profile for a particular measurement will be the retrieved temperature profile from the previous measurement. However, the *a priori* error variance is specified such that the solution error variance is dominated by measurement error (noise) over the range of altitudes where the signal-to-noise ratio is 10 or more. In effect, the weighting of *a priori* data is small over the altitude region where one can reasonably expect an accurate and precise retrieval from a direct measurement, and large enough outside of this altitude region to ensure a stable solution

In the outer relaxation loop, the pressure profile is rebuilt from the lower boundary using the onion-peel retrieved T_k profile and the barometric pressure law. The vibrational temperatures are updated using the CO_2 15 μm T_v model with the previously retrieved T_k and pressure profiles as input. The onion-peel retrieval (inner) loop is repeated until the entire inferred T_k profile relaxes within the convergence criterion, which is a requirement that the retrieved temperature profile differences between two successive onion-peel retrieval iterations be smaller than a user-specified fraction (same as above) of the solution error at a user-specified altitude. The user-specified altitude is chosen such that the signal-to-noise ratio is roughly 10 (typically, 110 to 115 km).

The top of the atmosphere (TOA) is nominally taken to be 140 km. This choice of TOA eliminates upper boundary effects on retrieved temperatures at altitudes where one can reasonably expect quality retrievals.

The non-LTE retrieval algorithm typically requires no more than five iterations in either (inner/outer) loop of the relaxation scheme. The algorithm can retrieve T_k at 51 tangent altitudes in 20 seconds on a desktop (500 Mhz Pentium) computer.

Results and Discussion

We now present retrieved temperature profiles from simulated SABER measurements and give estimates of the accuracy and sensitivity of the retrieved temperatures to parameters in the non-LTE model. The retrieval simulations were done on a 2 km grid, consistent with SABER's effective field-of-view. Shown in Figure 1 is a retrieval for a realistic temperature profile with two mesospheric inversion layers. This profile was derived from lidar measurements taken during the ALOHA 93 campaign [*Dao et al.*, 1995]. The first guess profile used to initialize the retrieval was an MSIS temperature profile, also shown in Figure 1. For the ALOHA case, the temperature profile is retrieved mostly within 3 K accu-

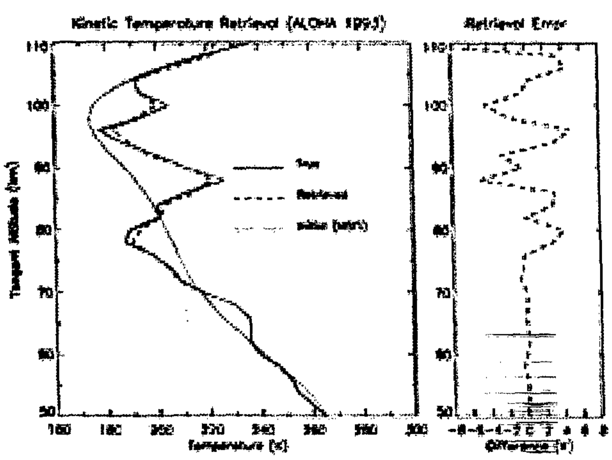

Figure 1. Simulated retrieval of kinetic temperature as measured by the SABER instrument for an atmosphere (ALOHA 93) with significant vertical structure.

Table 1. Determinations of k_o from laboratory measurements and as inferred from atmospheric observations

Laboratory Measurements			Atmospheric Observations	
Rate[a]	Temperature[b]	Reference	Rate[a]	Reference
1.4×10^{-12}	300	*Shved et al.* [1991]	6.0×10^{-12}	*Sharma and Wintersteiner* [1990]
1.2×10^{-12}	300	*Pollack et al.* [1993]	$3\text{-}6 \times 10^{-12}$	*López-Puertas et al.* [1992]
0.5×10^{-12}	301	*Lilenfeld* [1994]	1.5×10^{-12}	*Vollman et al.* [1997]

[a]Unit is $cm^{-3}s^{-1}$
[b]Unit is Kelvin

racy below 105 km, with the exceptions of a $\sim$ 5 K error at 88 and 96 km and a $\sim$ 4 K error at 80 and 100 km. Note also in Figure 1 the initial guess MSIS temperature profile has no small-scale atmospheric structure and differs from the lidar ("true") temperature profile by more than 35 K at some altitudes.

In the retrieval simulations presented above, the only sources of uncertainty included are simulated random instrument noise and calibration errors. There are other uncertainties to consider in a retrieval under non-LTE conditions. Specifically, CO_2 is apparently not well mixed above 75 km [*López-Puertas et al.*, 1998b]. Uncertainties in CO_2 will manifest themselves as uncertainties in the retrieved mesospheric temperature. In addition, uncertainties in the kinetic and spectroscopic parameters used in the computation of CO_2 T_v's will also contribute to uncertainties in the retrieved T_k. Certainly the most important of these parameters is the rate of physical quenching of CO_2 vibrations by collisions with atomic oxygen through the process

$$CO_2(01^10) + O \xrightarrow{k_o} CO_2(00^00) + O + 667\ cm^{-1}. \quad (1)$$

This process is critical to determining the T_v of the CO_2 ν_2 fundamental band in the upper mesosphere and lower thermosphere. The retrieved temperature profile depends on knowing the rate coefficient for this process (which we will call k_o) and the atomic oxygen concentration. There have been several determinations of k_o from which the rate has been inferred. The reported rate coefficients span the range from $0.5 \times 10^{-12}\ cm^3s^{-1}$ at 301 K determined by *Lilenfeld* [1994] to $6 \times 10^{-12}\ cm^3s^{-1}$ at 300 K inferred by *Sharma and Wintersteiner* [1990]. Table 1 lists the published values of the determinations of k_o. The temperature dependence of k_o is not known from laboratory measurement.

For the following sensitivity studies, we assume a 50% uncertainty in atomic oxygen and in k_o. We note that the SABER experiment will simultaneously measure the CO_2 abundance and that a number of techniques will be used to infer the atomic oxygen concentration (e.g.,

Table 2. Uncertainties in retrieved kinetic temperature (K) due to the specified uncertainty in the rate of physical quenching (k_o) of CO_2 vibrations by atomic oxygen (or equivalently, to uncertainty in atomic oxygen concentration) and due to the uncertainty in the CO_2 concentration (as described in the text). The uncertainty due to random instrument noise is in the column labeled "Noise". The column labeled "Cal" denotes the radiometric calibration error. The column "Total" is the root-sum-square of the uncertainty due to the previous 5 columns.

		Retrieval Uncertainty (K)					
Z(km)	T(K)	k_o(+50%) or [O]	k_o(-50%) or [O]	[CO_2]	Noise	Cal(1.7%)	Total
110.0	240.0	-7.4	16.3	7.6	11.3	-0.3	22.5
108.0	223.2	-6.0	14.2	4.5	6.9	0.1	17.5
106.0	212.8	-4.9	12.1	2.1	4.4	0.3	13.9
104.0	205.3	-3.9	10.0	0.8	5.7	0.4	12.2
102.0	199.5	-3.1	8.1	0.8	4.5	0.3	9.8
100.0	195.0	-2.4	6.4	1.4	3.5	0.2	7.8
98.0	191.7	-1.8	4.9	2.2	2.1	0.2	6.0
96.0	189.3	-1.2	3.6	2.9	2.6	0.2	5.4
94.0	187.7	-0.7	2.4	3.4	2.1	0.2	4.7
92.0	186.9	-0.3	1.4	3.6	1.4	0.2	4.1
90.0	186.8	-0.1	0.8	3.6	1.8	0.2	4.1
88.0	187.4	0.1	0.4	3.4	1.8	0.3	3.9
86.0	188.9	0.1	0.1	3.1	1.3	0.3	3.4
84.0	191.4	0.1	0.1	2.6	1.1	0.4	2.9
82.0	194.7	0.1	0.0	1.9	0.6	0.4	2.0
80.0	198.6	0.0	0.1	1.3	0.4	0.4	1.4

[*Mlynczak*, 1995]). The uncertainty in CO_2 is represented using two different CO_2 vmr profiles. The "true" CO_2 profile is assumed to be the profile taken from a rocket measurement described by *Wintersteiner et al.* [1992]. Temperature was retrieved using a CO_2 profile derived from ISAMS measurements [*López-Puertas et al.*, 1998b]. The two CO_2 profiles differ from one another between 70 and 110 km, with a maximum difference of $\sim$ 15% at 95 km. Shown in Table 2 are the results of this sensitivity study for a smoothed version of the US Standard Atmosphere. A goal of the SABER experiment from the outset has been to retrieve temperature to better than 3 K below 100 km in order to compute accurately the energy balance and dynamics of the mesosphere. Uncertainty in CO_2 dominates the error in retrieved temperature below 100 km. However, if the CO_2 abundance is simultaneously retrieved with sufficient accuracy, then uncertainties in atomic oxygen and k_o on the order of 50% or greater start to affect our ability to meet the SABER retrieval-uncertainty goal above about 90 km. In contrast, recall the order-of-magnitude range in the reported values for k_o. This goal can be achieved if the instrument performs on orbit as calibrated in the laboratory and if the non-LTE model and atmospheric parameters are known to accuracies better than indicated in Table 2.

Summary

We have presented an overview of a new algorithm for the rapid and accurate retrieval of T_k from measurements of CO_2 15 μm earth limb emission under non-LTE conditions. The algorithm faithfully recovers atmospheric temperature to better than 3 K accuracy for realistic atmospheres and runs in approximately 20 seconds on desktop computer hardware.

We note that in order to realize the potential of this algorithm (and hence, the SABER experiment) the range of uncertainty in k_o must be significantly reduced. We recommend a critical evaluation of the extant determinations by the chemical kinetics community. It would also seem prudent to quantify the dependence of this rate coefficient on temperature over the range commonly encountered in the MLT.

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